

Speculative Approaches to the
Mathematical Modelling of One Dimensional
P-N Junctions

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Summary

The one dimensional off state P-N junction is considered from the point of view of efficient numerical and in particular finite element analysis. The equations are briefly stated and specialised to the off state form. The known features of the solutions to the normalised equations are discussed. A number of finite element techniques developed in other applications during recent years are discussed, in a speculative way, to see if any might be advantageous in the P-N junction problem. The intention is to identify efficient finite element techniques which would then be applicable in more complicated problems, up to three dimensional on state transient devices.

1. Introduction

In recent years it has become accepted that the accurate numerical modelling of semi-conductor devices is an area of great importance, as it leads to a greater understanding of device behaviour and improved device efficiency. This is reflected in recent conferences devoted to this topic (NASECODES 1,2 and 3), [1,2,3] numerous publications in this area, see for example [36], and the setting up of an EEC initiative in device modelling.

In this paper an attempt is made to look at an extremely simple device, namely a P-N junction, considered in only one dimension. One of the problems of modelling semi-conductors is their highly non-linear behaviour. In the simpler off-state this occurs particularly at the joint between the P and N regions. In the on-state the rapid variation in the field variables can occur at an unknown place in the device. It was decided to concentrate in the first instance on the junction between P and N regions, to see if techniques could be evolved to give computationally cheap numerical solutions in one dimension. If this turned out to be possible, it was hoped that the methods could be extended to the on-state and to two and three dimensions.

The methods which will be looked at come from other finite element application areas, and are :

- grading and adaptive refinement of meshes
- mapping, global or local
- special finite elements with analytical expressions
- singularity techniques
- upwinding (Petrov-Galerkin) methods
- global elements
- boundary integrals
- shock or front modelling

It is of course possible that none of these techniques will work, but it does seem to be worth while to investigate them as there is no a priori reason to suppose that the classical polynomial interpolation and weighting is going to be the optimal finite element technique for such a non-linear problem. Moreover even if the proposed methods are not directly applicable they may suggest new possibilities which will work.

The techniques can be conveniently summarised as follows. The starting point is the off state differential equation which can be written as (details are given later)

$$f(\psi) = 0$$

This can be discretised as

$$\int \mathbf{W} f(\mathbf{N} \mathbf{U}) d\Omega = 0 \quad 2$$

In which \mathbf{U} is the electrostatic potential

\mathbf{N} is the element shape function

\mathbf{W} is a weighting function

Ω is the problem domain

and a summation over all elements is implied.

Mapping globally corresponds to changing Ω to a more convenient form.

Mapping locally corresponds to changing $\mathbf{N}(x,y)$ to $\mathbf{N}(x',y')$ where the mapped co-ordinates are x and y .

Using analytical expressions in the shape function corresponds to changing \mathbf{N}

Using Petrov Galerkin weighting corresponds to changing \mathbf{W}

Use of boundary integrals corresponds to the change of the domain from 2 dimensions to 1, and the use of different shape functions. (These should now be based on Green's functions, which are not available for non-linear problem.)

Many combinations of these possibilities exist.

2. Governing Equations

See, for example, Shockley[4] or Sze[5]. Poisson's equation for the electrostatic potential \mathbf{U} is

$$\nabla^2 \mathbf{U} = - \rho / \epsilon \quad 3$$

where ϵ is the dielectric permittivity and ρ , the space charge density is composed of two different mobile carrier densities (electrons, n and holes, p) and the doping of ionized donors and acceptors, N_D and N_A . So that

$$\rho = q (p - n + N_D - N_A) \quad 4$$

where q is the electron charge. n and p are given, in terms of quasi Fermi potentials for electrons and holes, ϕ_n and ϕ_p , as

$$p = n_i \exp q \left(\frac{\phi_p - \mathbf{U}}{kT} \right) \quad n = n_i \exp q \left(\frac{\mathbf{U} - \phi_n}{kT} \right) \quad 5$$

where T is absolute temperature and k is Boltzmann's constant.

The equations of hole and electron current continuity can be written as

$$\frac{\partial p}{\partial t} = - \frac{1}{q} \nabla \cdot \mathbf{J}_p - R \quad 6$$

$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_n - R \quad 7$$

and the equation for hole and electron currents is

$$\mathbf{J}_p = - q \mu_p p \nabla \psi - q D_p \nabla p \quad 8$$

$$\mathbf{J}_n = - q \mu_n n \nabla \psi + q D_n \nabla n \quad 9$$

in the above μ_n and μ_p are the electron and hole mobilities and D_n and D_p are the electron and hole diffusivities. R is the recombination and \mathbf{J}_n and \mathbf{J}_p are the hole and electron currents. A number of choices are available to the numerical modeller, n and p can be written in terms of the quasi-Fermi potentials ϕ_n and ϕ_p , equations 5. Other variables which can be used are η and ρ , where

$$\rho = \exp(q\phi_p/kT) \quad \text{and} \quad \eta = \exp(-q\phi_n/kT) \quad 10$$

It is worth noting that similar equations to those of the semi-conductor also arise in the study of reaction kinetics and that they have been successfully modelled using finite elements. [16,17,18,19] Similar equations also occur in the surface chemistry of clay minerals. In the reaction kinetics application questions of uniqueness and existence arise, which does not seem to be the case with semiconductors, presumably because the boundary conditions are different.

3. Nature of the solution

The classical one dimensional P-N problem has a solution whose form can be determined with a fair degree of precision, depending upon the doping.[6] The solution is characterised by a boundary layer effect at the junction between the P and N materials. It is possible to model the boundary layer directly, by using a very fine mesh of finite elements and this appears to be the only approach which is considered in the literature. However the consequences of this approach are as follows.

1. Fine meshes with very many unknowns.
2. Slow convergence.

4. Possible modelling techniques

It seems appropriate to ask if the modelling of the interface effects could not be made more efficient by improving the modelling. The main possibilities are as follows:

4.1 Grading or adaptive refinement of the mesh. Refinement is almost the only technique which has been used to date in the literature and has already been discussed. Adaptive refinement is a very interesting possibility which does not appear to have been used.

4.2 Mapping of co-ordinates. This method has been used in other numerical applications, chiefly as a means of dealing with very large or infinite domains. In these cases some means of extending the mesh is sought. The mapping can be global, [20] that is of the whole problem domain, or local to an element. [11]

4.3 Incorporation of analytical expressions in the finite element shape functions. For certain special values of the doping, an analytical solution to the off-state equation is known. It is possible to assume that the form of the solution for other doping functions will be reasonably similar to those known analytically. It is possible to include these known functions in the element shape function, along with the standard polynomials, which allow a measure of variation in the details of the device behaviour.

4.4 Singularity techniques. In elasticity problems singularities sometimes arise. Economical and efficient techniques have been devised for dealing with them. [7,8,15] In some respects the behaviour of the P-N junction can be regarded as very similar to that of the elasticity problem with a singularity. It might be thought that the connection between the two problems is fairly tenuous, but the benefits, should the techniques prove to be portable are potentially vast.

4.5 Upwinding or Petrov-Galerkin Methods. Boundary layers of the type that arise in the P-N junction also occur in fluid mechanics, which is where the term comes from. And the fluid mechanics method of matched asymptotic expansions has been used by Plesch [6] to arrive at P-N junction solutions. In recent years fluid mechanics problems in which boundary layers arise have been treated very effectively using 'upwinding' methods which are now, after considerable research, well understood. The same approach may be applicable in the analysis of P-N junctions.

5. Detailed assessment of the methods

5.1 Grading and adaptive refinement of meshes

There is nothing particularly subtle or complicated about the concept of grading the finite element mesh. It should be pointed out that the method will be most effective if the likely form of the analytical solution, and the element shape functions are both considered while generating the mesh. The

method can be linked to adaptive mesh generation, [21,23,24] which cannot be explored in depth here. In carrying out adaptive mesh refinement it is desirable, though not essential, that a suitable norm exist. It seems that in the off state case, or in the solution of the equation for electrostatic potential in a Gummel type of iteration, such a norm does exist. This will now be shown.

The governing equation, assuming ϕ_n and ϕ_p to be known functions of position can be written

$$\nabla^2 \psi = \gamma_1 \exp(\psi) + \gamma_2 \exp(-\psi) + \gamma_3 \quad 11$$

where γ_1 , γ_2 and γ_3 depend only upon position. The variational form of eqn. 11 can be written as

$$G = \int_{\Omega} F \, d\Omega \quad \text{where} \quad 12$$

$$F = \frac{1}{2} (\nabla\psi)^2 + \gamma_1 \exp(\psi) - \gamma_2 \exp(-\psi) + \gamma_3 \psi \quad 13$$

since the Euler-Lagrange equation corresponding to stationarity of G is

$$\frac{\partial F}{\partial \psi} - \frac{\partial F}{\partial(\partial\psi/\partial x)} - \frac{\partial F}{\partial(\partial\psi/\partial y)} = 0 \quad 14$$

which is just eqn. 11. The Legendre condition for the stationarity of G corresponding to a minimum is [12, p 215].

$$\frac{\partial^2 F}{\partial(\partial\psi/\partial x)^2} + \frac{\partial^2 F}{\partial(\partial\psi/\partial y)^2} > 0 \quad 15$$

which is clearly true for the functional, 13, so the exact solution of 11 corresponds to a minimum in G. This can be used to compare solutions, and to rank them in order of accuracy. In particular it provides a criterion when searching for optimal mappings.

Where no such variational form is available the adaptation of the mesh must proceed using some less precise criterion based on gradients of the potential.

5.2 Mapping Co-ordinates

Here it is necessary to map the narrow boundary layer region close to the junction into a much wider region, so that the details of the device behaviour can be resolved more sharply, and the gradients of the potential in the mapped model are not so steep and do not therefore generate such pronounced modelling difficulties. The general form of the desired mapping

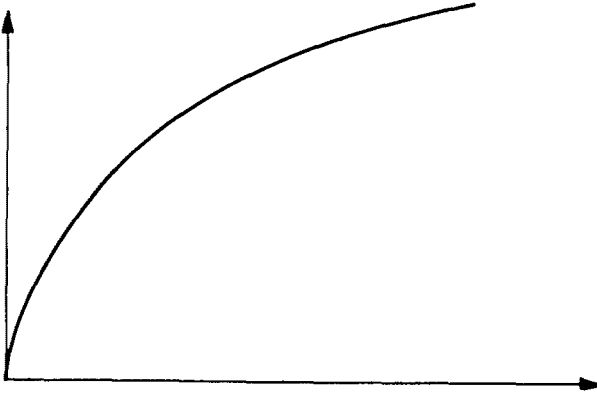


Figure 1. Approximate mapping function

is readily specified, and is as shown in Figure 1. If the problem is scaled in such a way that the width of the boundary layer in both sets of co-ordinates is 1 then the mapping must expand the first half of r , the real co-ordinate, into most of s , the mapped co-ordinate. There are an infinite number of possibilities here but two of them are :

5.2.1 A simple polynomial mapping of the form

$$s = \sqrt[n]{r} \quad 16$$

or, more generally

$$r = s^n \quad 17$$

where n is less than 1.

This can of course also be used as the basis of an economical and efficient mesh grading scheme.

5.2.2 A logarithmic scheme

$$s = \ln(r+1), \quad r = \exp(s) - 1 \quad 18$$

Many other possibilities exist. The form of the constant doping PN junction solution for potential is very like $\tanh(x)$ and so a mapping based on a hyperbolic function, particularly \tanh , might be effective here.

5.3 Analytical Expressions

For the case of constant doping it is possible to reduce the solution of the off-state potential equation to the

determination of an integral. This integral, although not available analytically, can be found to any desired accuracy, by the use of numerical quadrature. When doping is zero (not too important), there is an analytical solution and when doping is an arbitrary function of x the solution of the differential equation is more difficult. For the constant doping case the solution to the equation can now be treated as a function and it can be approximated. This function can now be used as the basis for a special element, in which the shape function is composed mainly of the special function, but with polynomials in addition. Suppose that we denote the constant doping solution by $PN(x)$. Then a suitable element shape function might be $PN(x)p(x)$, where $p(x)$ is a polynomial of desired degree. The element matrix can be formed in the usual way, with the derivatives of $PN(x)$ and $p(x)$ being readily obtained. The element shape function can be written

$$N(x) = PN(x) p(x) \quad 19$$

$$\text{and so } \frac{dN(x)}{dx} = \frac{dPN(x)}{dx} p(x) + \frac{dp(x)}{dx} PN(x) \quad 20$$

The next step is the integration over the element domain. This would be possible using a modest number of Gauss-Legendre integration points, or if more accuracy for less computational cost were required, a special quadrature formula could be developed. In any event provided that the function $PN(x)$ and its derivatives were available, no special problems should arise.

Such methods have already been applied in stress singularity problems of fracture mechanics to derive special elements which are very effective.[7,8] They have also been used to develop infinite elements for unbounded domains [9,10,11] and Hughes[14] has discussed in general terms the development of special elements for special problems.

Of course special shape functions have in a sense been used since the earliest attempts to model semi-conductor devices. The well-known Scharfetter-Gummel method [22,36] utilises a non linear shape function for the quasi-Fermi potentials. If a polynomial representation of ϕ_p is used in the hole continuity equation

$$\mu W J(\exp(-\phi) \nabla \rho) = R \quad 21$$

this leads to an exponential current density distribution close to each grid point. However this is a poor approximation, since current density varies only weakly with position. A good discussion of this point is given by Engl[36]. Requiring constant current density leads to a representation in which the nodal variable is $\exp(q\phi_p/kT)$, and the shape functions are nonlinear. The idea of a special shape function is also implicit in the presentation of Mock[37] in particular pages

58-60. It may be that a more formal acknowledgement of the use of special shape functions for all field variables, might lead to a more consistent and logical development and in particular, more rational generalisations to 2 and 3D problems. Another way of interpreting the Scharfetter Gummel algorithm is as a Petrov-Galerkin method.

A major question here is whether the function $PN(x)$ would change substantially if the doping were altered. If this were so, then the labour of recomputing the analytical solution for every change in the doping profile, might tell against such an approach. Simple analyses of junctions with abrupt changes and linear changes in doping [5] give quite similar distributions of potential. Another question is how this technique would extend to the two-dimensional case. In the first instance, one would envisage the special shape functions being used in the direction normal to the line of the boundary between P and N regions with conventional polynomial shape functions parallel to the boundary. However, where the PN boundary turns through a right angle, it is not clear what the best technique would be.

At present one cannot envisage how such a method would work, but one can outline a natural progression to evaluate the method.

1. Determine the ψ distribution for various constant dopings, using quadrature.
2. Repeat 1. for other doping distributions, including linear and quadratic variations, and those likely to occur in practise e.g. error function type distribution.
3. Study solutions from 1 and 2 for any common features. If the solutions are reasonably similar the technique may work, if not, it probably will not.
4. Assuming 3 is favourable devise a function $PN(x)$, which describes 'reasonably' the ψ distribution close to the junction.
5. Develop an interface element using the $PN(x)$ function normal to the interface and Gauss-Legendre quadrature.
6. If 5. works develop special quadrature formula, for higher accuracy. Some work has been done on this, for exponential shape functions, which seem a likely candidate, by Emson and Greenough [13].

An input from work on analytical solutions will clearly be of value in this area.

5.4 Singularity Techniques

In the case of elasticity it has been shown that for the 8 node iso-parametric finite element, a displacement of the midside node to the quarter point of the element edge induces a singularity in the mapping between the local and global co-ordinates, at the nearest vertex. This is easily seen by plotting the global co-ordinate, x as a function of the local co-ordinate, ξ , as shown in Figure 2. This was originally thought to be a totally undesirable feature of element behaviour, but Henshell[15] later showed that it could be exploited to enable the element to model accurately stress singularities.

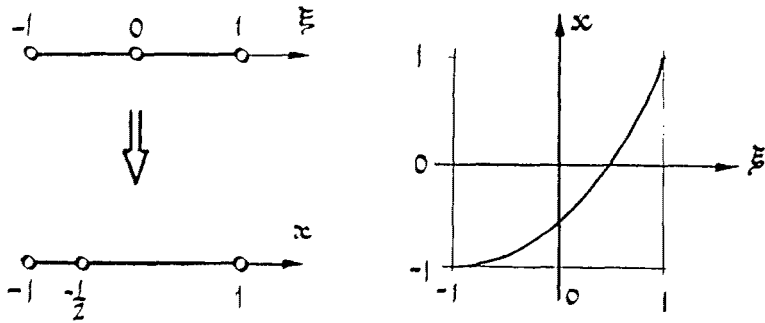


Figure 2 Singularity in x - ξ mapping induced by moving midside node to quarter point.

The rapid changes in the potential at the PN junction are not singular, but nevertheless this method may still be applicable. Firstly it is possible to make the mapping only tend towards singularity, by moving the node only part of the way towards the quarter point. This enables the element shape functions to model the rapid changes in potential more accurately without the presence of a true singularity. Secondly it is possible to use a different mapping function, instead of the original element shape function. This would follow the transfinite element techniques of Gordon and Hall.[25,26] It would be simple to devise a blending function, of the kind which they describe, which gives a linear mapping for midside nodes placed centrally, but which gives a suitable non-linear mapping as the node is moved away from the central position. The details of this have not been worked out yet, but no problems are envisaged.

Preliminary studies of the first option above, that is simply moving the midside node, towards the quarter point indicate that the modelling of the potential distribution, using only one element is greatly improved. The empirically determined optimal position for the test case was at about $x = -0.3$, where the two end nodes are at -1.0 and $+1.0$. Although

this has not been done yet, the functional given in eqn. 13 affords a way of selecting the best position for the middle node. Figures 3 to 6 show some potential distributions in half a symmetrical P-N junction in the equilibrium off state, in which the middle node has been moved to various positions.

No difficulties are envisaged when the line of the junction is not parallel to the side of the element, as it would simply mean moving the centre nodes on two adjacent edges, by distances which would be easy to compute. Clearly it would be unwise to expect too much from such a computationally crude device as this, but it is still worth considering, because the extra computational cost is virtually zero.

5.5 Upwinding or Petrov-Galerkin Techniques

These techniques have developed from efforts to solve the Navier-Stokes equations which govern viscous flow. They were originally an attempt to reproduce the finite difference method in which the differencing is not symmetrical, but is skewed in the 'upwind' direction. There has been a certain amount of controversy about the use of the methods, principally because they are alleged to introduce artificial dispersion. [39] It is now widely accepted that they are efficient and accurate. In the finite element context the method corresponds to using a special weighting function, which is different from the shape function. In this form it is termed the 'Petrov-Galerkin' method. [27,28,29,30]

The difficulty in modelling Navier-Stokes flows manifests itself chiefly in a narrow boundary layer. Because some of the difficulties in PN junction modelling also occur in a narrow boundary layer it seems natural to ask whether the same, or similar 'Petrov-Galerkin' weighting techniques might be effective, despite the dissimilarity in the structure of the governing equations.

The best argument in favour of the use of upwinding for the electrostatic potential is the close similarity in the general form of the solution to the normalised 1D P-N junction equation

$$\frac{d^2 \bar{\psi}}{dx^2} = 2 \sinh \bar{\psi} + \lambda \quad 22$$

subject to the boundary conditions $\bar{\psi}(0) = 0$ and $\bar{\psi}(1) = \bar{\psi}_0$, where $\bar{\psi}_0$ is the potential at the end of the device, and the 1D convective diffusion equation.

$$\frac{d^2 \phi}{dx^2} + \alpha \frac{d\phi}{dx} = 0 \quad 23$$

This has the analytical solution

$$\phi = (1 - \exp(-\alpha x)) / (1 - \exp(-\alpha)) \quad 24$$

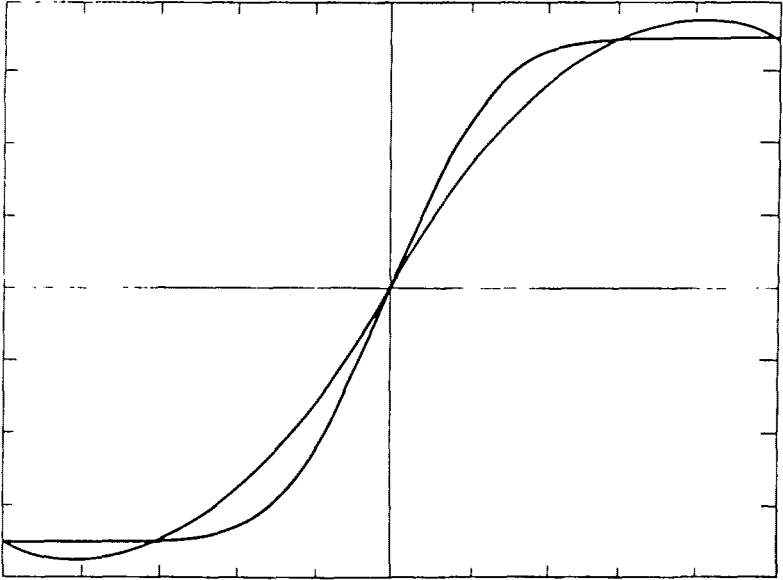


Figure 3 PN junction analysis 2, 3 node quadratic finite elements. Central node in each element at $x = 0.0$

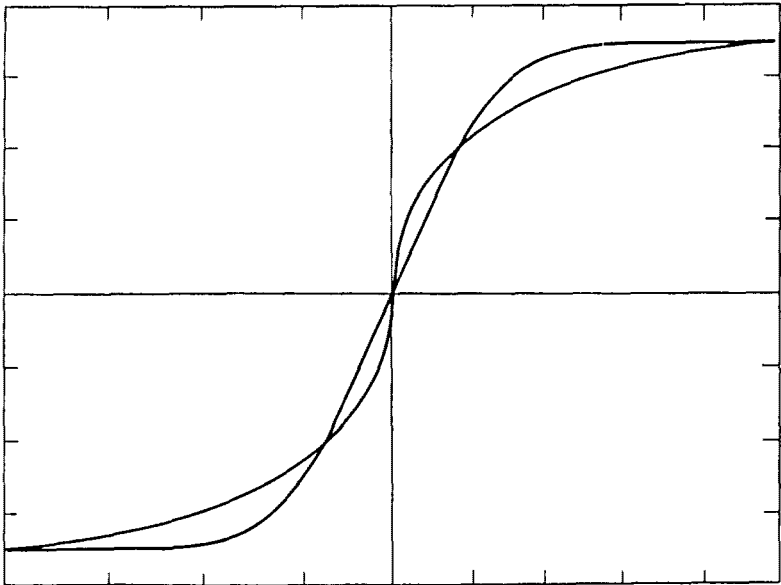


Figure 4 PN junction analysis 2, 3 node quadratic finite elements. Central node in each element at $x = -0.5$

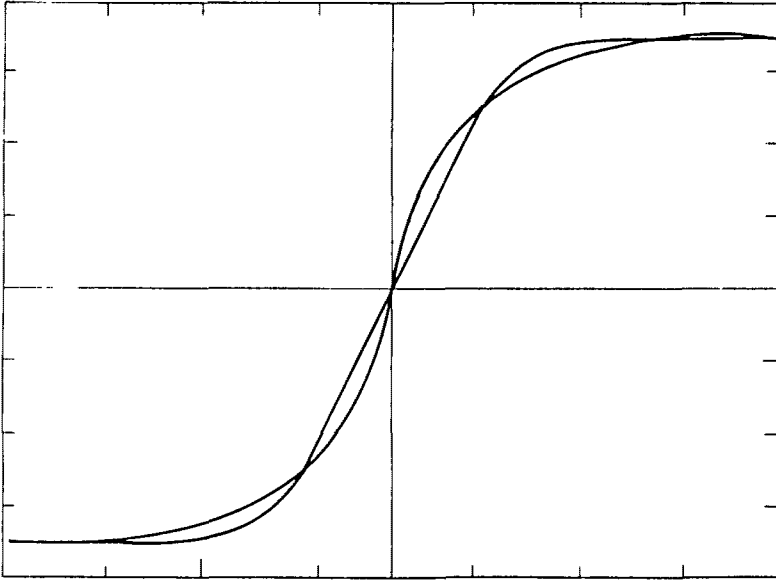


Figure 5 PN junction analysis 2, 3 node quadratic finite elements. Central node in each element at $x = -0.4$

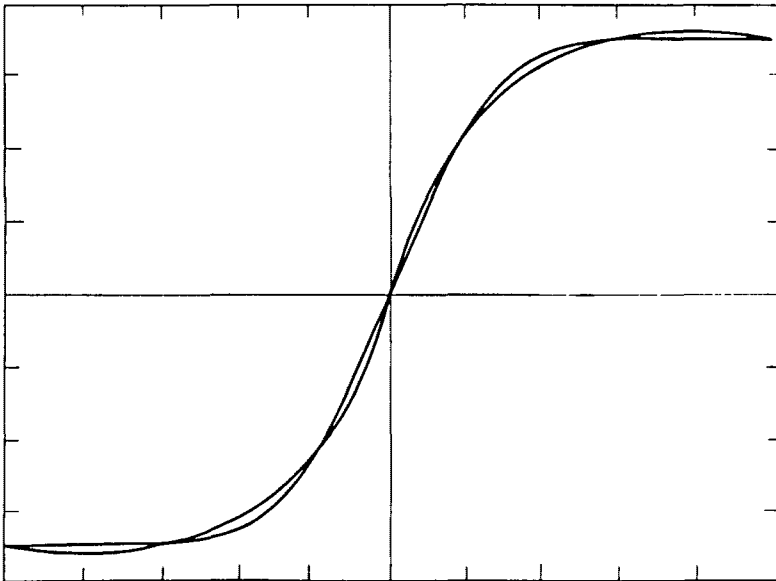


Figure 6 PN junction analysis 2, 3 node quadratic finite elements. Central node in each element at $x = -0.3$

Clearly eqn. 23 is linear, whereas eqn. 22 is non linear, and the equation structure is completely different. However, the similarity in the solutions shown in Figs. 7,8 and 9 is striking. Both are essentially boundary layer effects.

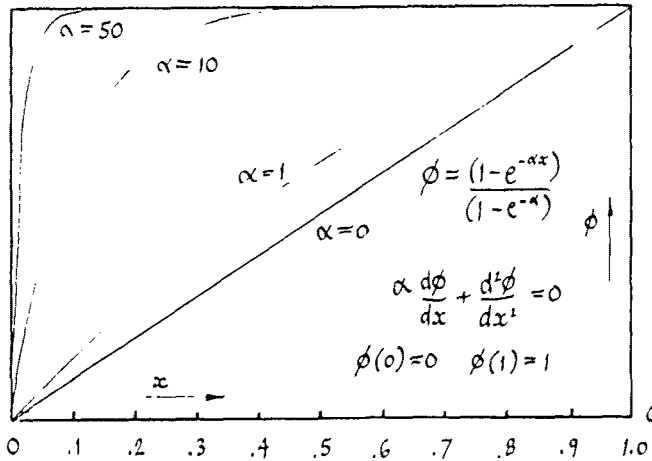


Figure 7 Analytical Solutions for Convective Diffusion Equation

Figures 8 and 9 show the solution for electrostatic potential for 2 different dopings, for uniformly divided and for graded finite element meshes. For higher doping, and a uniform mesh, the finite element (Galerkin) results show some oscillations. However these oscillations are not of the same type as those in the convective diffusion problem, and there is no theoretical reason why an upwinding process should work.

Upwinding, or the Petrov-Galerkin method, has certainly been successful in handling problems in fluid mechanics, including Berger's equation and the Navier-Stokes equations, But there are theoretical results which suggest that for self-adjoint problems, the usual Galerkin weighting is optimal. The 1D equation 22 is not self-adjoint, at any rate in the classical definition, used by Courant and Hilbert[12] and Strang and Fix[40], but it does have a corresponding minimal problem as we have shown, which could imply that the Galerkin method will give the best results, in terms of the norm, though not possibly, the best nodal values.

When the current continuity equations are written in terms of the densities of electrons and holes, then if the electric field is viewed as constant, they fall into the category of convective-diffusion equations, as is remarked by Campbell[38]. As stated earlier, there is a virtual identity between optimal upwinding and the Scharfetter-Gummel algorithm. This suggests that the existing theory for extending Petrov-Galerkin to 2 or more dimensions may be very useful as a way of extending the Scharfetter-Gummel algorithm.

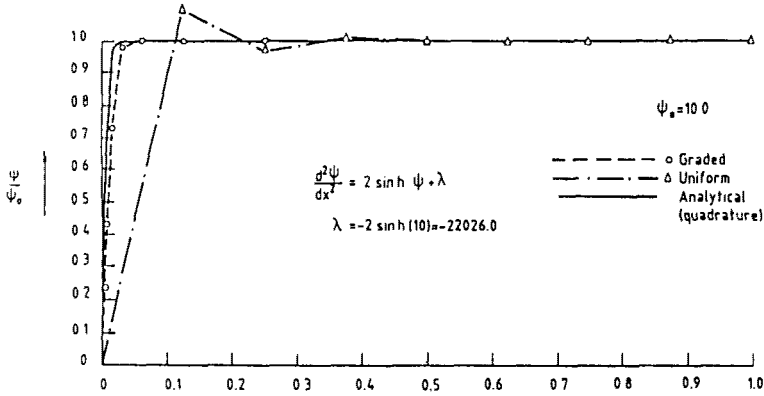


Figure 8 Half of PN junction - moderate doping

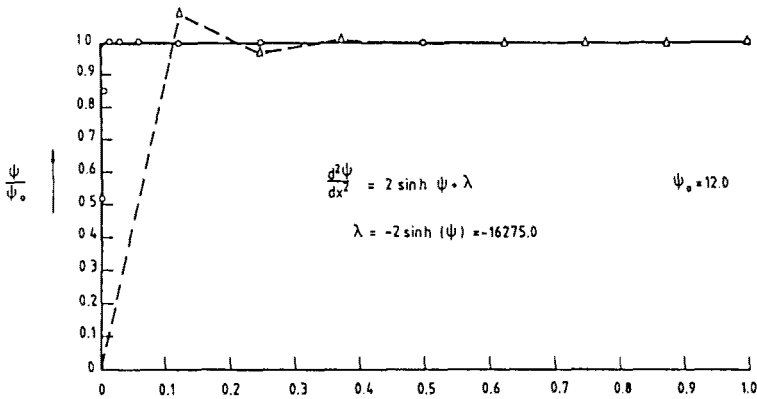


Figure 9 Half of PN junction - higher doping

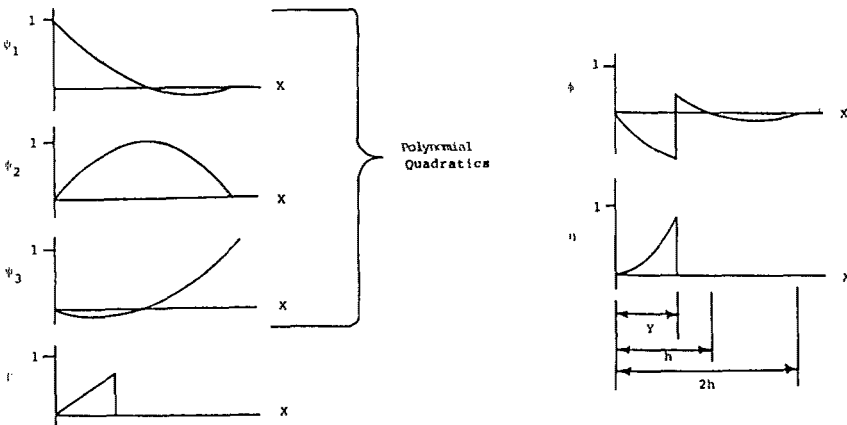


Figure 10 Discontinuous Shape Functions (Ref[32])

5.6 Shock and Front type modelling

Many of the more severe problems in semi-conductor device modelling arise in the on-state case, where the narrow 'boundary layers' in which there are rapid changes in potential and currents do not necessarily occur on junctions of material properties, and may, in the transient case, move about through the device. There is some experience in modelling other problems in which such 'fronts' or 'shocks' occur, using finite elements. They occur in secondary oil recovery and in underwater explosions to name but two applications. Techniques which have been adopted to date are as follows

1. Local refinement of the mesh at the shock. This is of course simply the method described earlier. However in addition the shock has now to be first found, and then tracked. A method for doing this in oil recovery problems is described by White.[31] As the location of the shock moves, it is also necessary to change the position of the refined section of mesh, and this brings problems of interpolation and extrapolation to the new mesh locations

2. Wellford and Oden[32] have proposed a special element for dealing with problems in which shocks occur. In this case the element formulation permits a shock of unknown size and position in the shape function. A shape function is shown in Fig. 9. This method has been extended by Stevens[33].

3. Finn[34] splits the advective and diffusion parts of the advective diffusion equation and advects the finite element mesh at the correct speed and then solves for diffusion only. The current continuity equations, in terms of n and p , might be amenable to this technique. However as elements have to be introduced and removed at the ends of the mesh, the house keeping problems, particularly in 2 and 3 dimensions are formidable.

Other recent developments in this area are given in [41,42].

6. Conclusions

This is a rapidly moving area, and it is difficult to predict which methods will prove to be the best. In our view the two most promising areas are special shape functions, and Petrov-Galerkin weightings.

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